An asymptotic form of the reciprocity theorem with applications in x-ray scattering

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Abstract

The emission of electromagnetic waves from a source within or near a non-trivial medium (with or without boundaries, crystalline or amorphous, with inhomogeneities, absorption and so on) is sometimes studied using the reciprocity principle. This is a variation of the method of Green's functions. If one is only interested in the asymptotic radiation fields the generality of these methods may actually be a shortcoming: obtaining expressions valid for the uninteresting near fields is not just a wasted effort but may be prohibitively difficult. In this work we obtain a modified form the reciprocity principle which gives the asymptotic radiation field directly. The method may be used to obtain the radiation from a prescribed source, and also to study scattering problems. To illustrate the power of the method we study a few pedagogical examples and then, as a more challenging application we tackle two related problems. We calculate the specular reflection of x rays by a rough surface and by a smoothly graded surface taking polarization effects into account. In conventional treatments of reflection x rays are treated as scalar waves, polarization effects are neglected. This is a good approximation at grazing incidence but becomes increasingly questionable for soft x rays and UV at higher incidence angles.

PACs: 61.10.Dp, 61.10.Kw, 03.50.De

1 Introduction

The principle of reciprocity can be traced to Helmholtz in the field of acoustics. It states that everything else being equal the amplitude of a wave at a point A due to a source at point B is equal to the amplitude at B due to a source at A. With its extension to electromagnetic waves by Lorentz [1] and later to quantum mechanical amplitudes [2], the applicability to all sorts of fields was made manifest. Nowadays the principle is regarded as a symmetry of Green's functions when the source point and the field point are reversed. This symmetry is actually quite general. As shown in [3] the conditions of time-reversal invari-

ance and hermiticity of the Hamiltonian are sufficient to guarantee reciprocity, but they are not necessary; in fact, reciprocity holds even in the presence of complex absorbing potentials. In the case of electromagnetic waves the only requirement is that the material medium be linear and described by symmetric permittivity and permeability tensors [4][5]. This excludes plasmas and ferrite media in the presence of magnetic fields.

In the field of x-ray optics the principle was used by von Laue [6] to explain the diffraction patterns generated by sources within the crystal, the so-called Kossel lines [7]. More recently there has been a widespread recognition that these interference patterns contain information not just about intensities but also about phases and can be thought of as holographic records from which real space images of the location of the internal sources can be reconstructed. Thus, under the modern name of 'x-ray holography' there has been a considerable revival of interest in this subject [8].

However, powerful as it is, the usual formulation of the reciprocity principle suffers from a rather serious drawback: it refers to the exchange of source and field *points*. As a consequence, a careful application of the principle requires one to consider the emission of spherical waves which in crystalline media or even in the mere presence of plane boundaries, can be surprisingly difficult (recall *e.g.* studying the radiation by an antenna in the vicinity of the conducting surface of the Earth [9] or of layered media [10]). Furthermore, one is typically interested in the asymptotic radiation fields so the relevant exchange should involve a source point *here* with a field point at *infinity*.

These technical difficulties have not deterred the users of reciprocity from using the principle to make valuable predictions, but a high price has been paid. The required asymptotic limits are usually taken *verbally* and no accounts are given of where and how spherical waves are replaced by plane waves. Such sleights of hand, because skillfully performed, have not lead to wrong results, but intensities are predicted only up to undetermined proportionality factors and this excludes applications to classes of problems where absolute intensities are needed. Moreover one is left with the uneasy feeling that the validity of the predictions is justified mostly on the purely pragmatic grounds that for the problem at hand they seem to work which, again, limits applications to problems that are already familiar.

The main goal of this paper (section 2) is to obtain a modified form of the reciprocity theorem that gives the asymptotic radiation fields directly and that accommodates plane waves and both point and extended sources in a natural way. Remarkably the resulting expressions, which include all the relevant proportionality factors and yield absolute, not just relative intensities, are very simple.

For many problems the Asymptotic Reciprocity Theorem (ART) obtained here represents an improvement not only over the usual form of the reciprocity theorem but also over the method of Green's functions. Computing the Green's function requires solving a boundary value problems for spherical waves in the presence of plane boundaries and/or periodic media; this may well be an intractably difficult problem. Furthermore, a considerable effort is wasted by first

obtaining both near fields and far fields and then discarding the uninteresting near fields. The ART is a shortcut that discards the near fields before, rather than after they are computed.

To illustrate the power of the method we consider several applications. The first three (section 3) are brief pedagogical examples of increasing complexity. First the ART is used to calculate the fields radiated by an arbitrary prescribed source in vacuum; next as an application to scattering problems we reproduce the kinematical theory of diffraction by crystals. The third example, the radiation by a current located near a plane dielectric boundary, is straightforward when the ART is used but not if other methods are used. One must emphasize that what is new in these examples are not the results, but the method; the first two are standard textbook material, a special case of the third is treated in [9]. As a more involved application of the ART, in section 4 we combine ideas from the three previous examples to study two other related scattering problems, the specular reflection of polarized x rays by a rough surface and by a continuously graded surface.

The technique of the grazing-incidence reflection of x-rays has received considerable attention [11]-[17] from both the theoretical and the experimental sides as a means to obtain structural information about surfaces. The effect of surface roughness on the reflection is taken into account by multiplying the Fresnel reflectivity of an ideal sharp and planar surface by a "static Debye-Waller" factor. The problem is to calculate this corrective factor. The calculation has been carried out in several different approximations. The Rayleigh or Born approximation [11] is satisfactory for rough surfaces with long lateral correlation lengths but for x-rays the situations of interest generally involve short lateral correlation lengths. Here other approximations such as the distorted-wave Born approximation [13][14] and the Nevot-Croce approximation [15] are used. For variations and interpolations between these two methods see [16], and for a generalization to surfaces with non-Gaussian roughness and to graded interfaces of arbitrary profile see [17]. In these treatments ([14] is an exception) the x rays are treated as scalar waves. One expects this approximation to hold at grazing incidence but at higher incidence angles (*e.g.*, for soft x rays) its validity becomes increasingly questionable. Using a modified first Born approximation Dietrich and Haase [14] took the vector character of the x rays into account but they point out that the validity of their approximation is not in general easy to assess and they restrict themselves to studying special interface profiles.

In section 4 we study this problem using a different approximation; we use the ART to develop approximations of the Nevot-Croce type [17]. There is, of course, a trivial polarization dependence that is already described by Fresnel formulas for the reflectivity of the ideal flat step surface. The question we address here is whether the "static Debye-Waller" factor shows any additional dependence on polarization. The final result is remarkably simple: the "static Debye-Waller" factor for the specularly reflected vector waves is the same for both polarizations and coincides with that for scalar waves. Finally, some brief concluding remarks are collected in section 5.

Figure 1: (a) In the usual form of the reciprocity theorem the surface S encloses the medium, and all sources. (b) For the asymptotic form of the reciprocity theorem the connecting field $\vec{E}_c$ is a radiation field, its source lies outside the surface $S = S_+ + S^{'}$.

2 The reciprocity theorem and its asymptotic form

We wish to calculate the asymptotic radiation fields $\vec{E}$ and $\vec{H}$ generated by a prescribed current $\vec{J}\,(t, \vec{r})$ located near or within a linear medium,

$$D_i = \varepsilon_{ij} E_j \quad \text{and} \quad B_i = \mu_{ij} H_j \ .$$

We will assume that the tensors $\varepsilon_{ij}\,(\vec{r})$ and $\mu_{ij}\,(\vec{r})$ are symmetric, but otherwise the situation remains quite general, the medium may have an irregular shape, or be inhomogeneous, crystalline or amorphous, absorbing, dispersive, etc.

As in the usual deduction of the reciprocity theorem (see *e.g.*, [4]), we consider a second set of fields $\vec{E}_c$ and $\vec{H}_c$, which we will call the "connecting fields", generated by a source $\vec{J}_c$ (see fig.1a). For simplicity we will also assume that all fields and sources are monochromatic $\vec{E} = \vec{E}(\vec{r})e^{-i\omega t}$, $\vec{J} = \vec{J}(\vec{r})e^{-i\omega t}$, etc. For linear media this is not a restriction.

From Maxwell's equations

$$\nabla \times \vec{E} = iK\vec{B} \qquad \text{and} \qquad \nabla \times \vec{H} = -iK\vec{D} + \frac{4\pi}{c}\vec{J}, \tag{1}$$

where $K \equiv \omega/c$, one easily obtains the following identity

$$\nabla \cdot \left(\vec{E} \times \vec{H}_c - \vec{E}_c \times \vec{H} \right) = \frac{4\pi}{c} \left(\vec{E}_c \cdot \vec{J} - \vec{E} \cdot \vec{J}_c \right),$$

which, on integrating over a large volume V bounded by the surface S, can be rewritten as

$$\int_S \left(\vec{E}\times\vec{H}_c-\vec{E}_c\times\vec{H}\right)\cdot d\vec{s}=\frac{4\pi}{c}\int_V \left(\vec{E}_c\cdot\vec{J}-\vec{E}\cdot\vec{J}_c\right)\,dv. \tag{2}$$

This expression simplifies if one deals with point sources. For example, consider oscillating point dipoles $\vec{p}_o e^{-i\omega t}$ and $\vec{p}_c e^{-i\omega t}$, located at $\vec{r}_o$ and $\vec{r}_c$ respectively. The current density $\vec{J}$ is given by $\vec{J}=-i\omega\vec{p}_o\delta\left(\vec{r}-\vec{r}_o\right)e^{-i\omega t}$ and $\vec{J}_c$ is given by an analogous expression. Further simplification is achieved if one assumes that the surface S is so remote that the surface integral is negligibly small [18], then

$$\vec{E}_c\left(\vec{r}_o\right)\cdot\vec{p}_o=\vec{E}\left(\vec{r}_c\right)\cdot\vec{p}_c\ . \tag{3}$$

This is the usual form of the reciprocity theorem; it says that if we know $\vec{E}_c$ at the location of $\vec{p}_o$ we can calculate $\vec{E}$ at the location of $\vec{p}_c$. This elegant result takes us a long way toward a final answer for $\vec{E}$, but the remaining problem of calculating $\vec{E}_c$, that is, the calculation of how the spherical wave generated by $\vec{p}_c$ is scattered by the medium, can still be too difficult.

A more useful version of the theorem can be obtained once one realizes that the connecting field is merely a tool that codifies information about the influence of the non-trivial medium. Above, the field $\vec{E}_c$ has been introduced by first specifying a source $\vec{J}_c$, but clearly this is an unnecessary additional complication. In fact, since the most convenient $\vec{J}_c$ is that which results in the simplest $\vec{E}_c$ it is best to focus attention directly on the field rather than its source. Thus we move $\vec{J}_c$ outside the surface S, to infinity (see fig.1b) so that throughout the volume V the connecting field $\vec{E}_c$ is a pure radiation field. Furthermore, let the surface S itself be so distant that on S itself both $\vec{E}$ and $\vec{E}_c$ are *vacuum* radiation fields. Then

$$\int_S \left(\vec{E}\times(\nabla\times\vec{E}_c)-\vec{E}_c\times(\nabla\times\vec{E})\right)\cdot d\vec{s}=\frac{4\pi iK}{c}\int_V \vec{E}_c\cdot\vec{J}\,dv. \tag{4}$$

At this point it is not yet clear that this form of the reciprocity theorem is simpler than eq. (3) but one remarkable feature can already be seen: eq. (4) relates the field $\vec{E}$ at a distant surface S to its source $\vec{J}$ within a nontrivial medium *without* having to calculate $\vec{E}$ in the vicinity of $\vec{J}$. The "connection" between the distant radiation field $\vec{E}$ and its source $\vec{J}$ is achieved through the much simpler (i.e., hopefully calculable) "connecting" field $\vec{E}_c$.

To bring eq. (4) into a form that is manifestly simpler than (3) the surface S is chosen as a cube with edges of length $L\to\infty$. In fig.1b the upper face, defined by a constant z coordinate, $z=z_+$, has been singled out as S_+, the remaining seven faces are denoted $S^{'}$.

On the upper face S_+ we write the field $\vec{E}$ as a superposition of outgoing plane waves of wave vector $\vec{k}$ satisfying $\vec{k}\cdot\vec{k}=\omega^2/c^2=K^2$ and $k_z>0$,

$$\vec{E}\left(\vec{r}\right)=\int\limits_{k_z>0}\frac{d^3k}{\left(2\pi\right)^3}\,2\pi\delta\left(k-K\right)\,\vec{E}(\vec{k})\,e^{i\vec{k}\cdot\vec{r}}\,, \tag{5}$$

where, in a self-explanatory notation, $\vec{k}\cdot\vec{r} = \vec{k}_\perp \cdot \vec{r}_\perp + k_z z_+$. It is here, by the very act of writing $\vec{E}$ in this form, that the asymptotic limit of discarding near fields is being taken. For $z << z_+$ additional terms describing the near fields should be included.

The integral over dk_z is most easily done using

$$\delta\left(k-K\right) = \frac{K}{k_z}\left[\delta\left(k_z - \sqrt{K^2-k_\perp^2}\right) - \delta\left(k_z + \sqrt{K^2-k_\perp^2}\right)\right]. \tag{6}$$

The result is

$$\vec{E}\left(\vec{r}\right) = \int \frac{d^2k_\perp}{\left(2\pi\right)^2}\,\frac{K}{k_z}\,\vec{E}(\vec{k})\,e^{i\vec{k}\cdot\vec{r}}, \tag{7}$$

where $k_z = +\sqrt{K^2-k_\perp^2}$.

The choice of the connecting field $\vec{E}_c$ is dictated purely by convenience. A particularly good choice for $\vec{E}_c$ is the superposition of an incoming plane wave of unit amplitude (we use $\hat{}$ to denote vectors of unit length) and wave vector $\vec{k}_c$, with $\vec{k}_c\cdot\vec{k}_c = K^2$ and $k_{cz} < 0$, plus all the waves scattered by the medium,

$$\vec{E}_c\left(\vec{r}\right) = \hat{e}_c\,e^{i\vec{k}_c\cdot\vec{r}} + \vec{E}_c^{'}\left(\vec{r}\right). \tag{8}$$

On S_+, the scattered field $\vec{E}_c^{'}$ is a superposition of outgoing plane waves and is given also in a form analogous to eq. (7),

$$\vec{E}_c^{'}\left(\vec{r}\right) = \int \frac{d^2k_\perp^{'}}{\left(2\pi\right)^2}\,\frac{K}{k_z^{'}}\,\vec{E}_c^{'}(\vec{k}^{'})\,e^{i\vec{k}^{'}\cdot\vec{r}}, \tag{9}$$

with $\vec{k}^{'}\cdot\vec{r} = \vec{k}_\perp^{'}\cdot\vec{r}_\perp + k_z^{'}z_+$ and $k_z^{'} = +\sqrt{K^2-k_\perp^{'2}}$.

Now we are ready to calculate the surface integral on the left hand side of eq. (4). Substituting (8) into (4) the integral over S_+ separates into two terms, one due to the incoming plane wave $\hat{e}_c\,e^{i\vec{k}_c\cdot\vec{r}}$, and the other due to the scattered waves $\vec{E}_c^{'}\left(\vec{r}\right)$. The first term is

$$I_1 = \int_{S_+} dx\,dy\,\hat{e}_z\cdot\left(\vec{E}\times(i\vec{k}_c\times\hat{e}_c) - \hat{e}_c\times(\nabla\times\vec{E})\right)e^{i\vec{k}_c\cdot\vec{r}}, \tag{10}$$

and substituting (7) its evaluation is straightforward. The integral over $dx\,dy$ yields $(2\pi)^2\delta(\vec{k}_\perp + \vec{k}_{c\perp})$. Since $k^2 = k_c^2 = K^2$, $k_{cz} < 0$ and $k_z > 0$ this implies that the plane waves superposed in (7) yield a vanishing contribution except when $\vec{k} = -\vec{k}_c$. Thus,

$$I_1 = -2iK\,\hat{e}_c\cdot\vec{E}(-\vec{k}_c) \tag{11}$$

The contribution of the scattered waves $\vec{E}_c^{'}\left(\vec{r}\right)$,

$$I_2 = \int_{S_+} dx\,dy\,\hat{e}_z\cdot\left(\vec{E}\times(\nabla\times\vec{E}_c^{'}) - \vec{E}_c^{'}\times(\nabla\times\vec{E})\right), \tag{12}$$

is calculated in a similar way. Substitute (7) and (9) and integrate over $dx\,dy$ to obtain a delta function. This eliminates all Fourier components except those with $\vec{k}_\perp = -\vec{k}'_\perp$. Since $k^2 = k^{'2} = K^2$, and both $k_z, k_z' > 0$ this implies $k_z = k_z' > 0$. Thus,

$$I_2 = \int \frac{d^2k_\perp'}{(2\pi)^2} \frac{K^2}{k_z'^2} \hat{e}_z \cdot \left[\vec{E}(\vec{k}) \times \left(i\vec{k}' \times \vec{E}_c'(\vec{k}') \right) - \vec{E}_c'(\vec{k}') \times \left(i\vec{k} \times \vec{E}(\vec{k}) \right) \right], \quad (13)$$

where $\vec{k} = -\vec{k}' + 2k_z'\hat{e}_z$. Further manipulation using $\vec{k}' \cdot \vec{E}_c'(\vec{k}') = \vec{k} \cdot \vec{E}(\vec{k}) = 0$ gives $\hat{e}_z \cdot [\cdots] = 0$, so that

$$I_2 = 0. \quad (14)$$

According to eq. (11) and (14) the only contributions to the surface integral over the distant plane S_+ come from products of outgoing with incoming waves. Products of two outgoing waves yield vanishing contributions. This result applies also to the remaining seven faces of the cube S. Since on each of these faces there are only outgoing waves we find that the integral over S' makes no contribution to the left hand side of (4). Incidentally, this argument completes our previously unfinished deduction of the usual form of the reciprocity theorem, eq. (3): if both sources $\vec{J}$ and $\vec{J}_c$ are internal to the surface S the surface integral in eq. (2) vanishes because it only involves products of outgoing waves.

Substituting (11) into (4) leads us to the main result of this paper, the asymptotic reciprocity theorem,

$$\widehat{e} \cdot \vec{E}(\vec{k}) = -\frac{2\pi}{c} \int_V \vec{E}_c \cdot \vec{J}\, dv. \quad (15)$$

In words:

The field $\vec{E}(\vec{k})$ radiated in a direction $\vec{k}$ with a certain polarization $\widehat{e}$ is $-2\pi/c$ times the "component" of the source $\vec{J}(\vec{r})$ "along" a connecting field $\vec{E}_c(\vec{r})$ with incoming wave vector $\vec{k}_c = -\vec{k}$ and polarization $\widehat{e}_c = \widehat{e}$.

Typically one is interested in the intensity radiated into a solid angle $d\Omega$; since the amplitude $\vec{E}(\vec{k})$ that appears in (7) and (15) is not quite the Fourier transform of $\vec{E}(\vec{r})$ it may be useful to derive an explicit expression for $dW/d\Omega$. The total power radiated through the plane S_+ is given by the flux of the time-averaged Poynting vector, $\frac{c}{8\pi}\,\mathrm{Re}\,[\vec{E} \times \vec{B}^*]$,

$$W = \int d^2x_\perp \frac{c}{8\pi}\,\mathrm{Re}\,[\vec{E} \times \vec{B}^*] \cdot \hat{e}_z = \int d\Omega\, \frac{dW}{d\Omega} \quad (16)$$

Using (7) and $d^2k_\perp = k_\perp dk_\perp d\phi = Kk_z d\Omega$ (where ϕ is the usual azimuthal angle about the z axis) we get

$$W = \frac{c}{8\pi} \int \frac{d^2k_\perp}{(2\pi)^2} \frac{K}{k_z} \vec{E}(\vec{k}) \cdot \vec{E}^*(\vec{k}), \quad (17)$$

so that

$$\frac{dW}{d\Omega} = \frac{c}{8\pi} \left(\frac{K}{2\pi} \right)^2 \vec{E}(\vec{k}) \cdot \vec{E}^*(\vec{k}). \quad (18)$$

In the next section we offer a few illustrative examples of the ART in action.

3 Some simple examples

The ART, eq. (15), holds for an arbitrary linear medium. In particular it holds if the medium is vacuum. Our first trivial example is the radiation by a prescribed current in vacuum. Next, to show that the ART can be used to study scattering problems we deal with another equally trivial example, the kinematical theory of diffraction by crystals. The third example, the radiation by currents located near a dielectric boundary, is also straightforward. What is remarkable here is the ease with which the results are obtained compared to conventional methods [9][10].

3.1 Radiation in vacuum

In this case the connecting field is just an incoming plane wave, $\vec{E}_c\,(\vec{r}) = \hat{e}_c\, e^{i\vec{k}_c\cdot\vec{r}}$. The ART, eq. (15), gives the radiated field with polarization $\hat{e} = \hat{e}_c$ as

$$\widehat{e}\cdot\vec{E}(\vec{k}) = -\frac{2\pi}{c}\int_V \vec{J}(\vec{r})\cdot\hat{e}\, e^{-i\vec{k}\cdot\vec{r}}\, dv = -\frac{2\pi}{c}\,\hat{e}\cdot\vec{J}(\vec{k}), \tag{19}$$

so that

$$\vec{E}(\vec{k}) = \frac{2\pi}{c}\hat{k}\times(\hat{k}\times\vec{J}(\vec{k})). \tag{20}$$

The radiated power, eq. (18), is

$$\frac{dW}{d\Omega} = \frac{K^2}{8\pi c}\left|\hat{k}\times(\hat{k}\times\vec{J}(\vec{k}))\right|^2, \tag{21}$$

as expected. (For radiation by a point dipole just substitute $\vec{J}(\vec{k}) = -icK\vec{p}$.)

3.2 Bragg diffraction

Consider a crystal described by its dielectric susceptibility $\chi(\vec{r})$ [19] which for x rays is quite small (typically about 10^{-5} or less). An incident plane wave $\vec{E}_o e^{i\vec{k}_o\cdot\vec{r}}$ induces a current

$$\vec{J}(\vec{r}) = -i\omega\vec{P}(\vec{r}) = \frac{-i\omega}{4\pi}\chi(\vec{r})\vec{E}_o e^{i\vec{k}_o\cdot\vec{r}}, \tag{22}$$

which radiates. The connecting field needed to calculate this radiation is a simple incoming plane wave, $\vec{E}_c\,(\vec{r}) = \hat{e}_c\, e^{i\vec{k}_c\cdot\vec{r}}$, and the ART, eq. (15), gives the radiated field as

$$\vec{E}(\vec{k}) = -\frac{i\omega}{2c}\hat{k}\times(\hat{k}\times\vec{E}_o)\,\chi(\vec{k}-\vec{k}_o). \tag{23}$$

The scattered field is proportional to the Fourier transform of the susceptibility of the medium; for a periodic medium this is Bragg diffraction.

3.3 Radiation in the vicinity of a reflecting surface

Consider a current $\vec{J}_{in}(\vec{r})$ located within a uniform medium with dielectric susceptibility χ_0 occupying the region $z<0$ (see fig. 2). To calculate the radiation in the direction $\vec{k}$ with polarization $\hat{e}$ we choose as connecting field an incoming plane wave with wave vector $\vec{k}_c = -\vec{k}$ and unit amplitude $\hat{e}_c = \hat{e}$ plus the corresponding reflected and transmitted waves,

$$\vec{E}_c(\vec{r}) = \begin{cases} \hat{e}_c \, e^{i\vec{k}_c\cdot\vec{r}} + \vec{\varepsilon}_{cr}\, e^{i\vec{k}_{cr}\cdot\vec{r}}, & \text{for} \quad z>0 \\ \vec{\varepsilon}_{ct}\, e^{i\vec{k}_{ct}\cdot\vec{r}}, & \text{for} \quad z<0 \end{cases} \tag{24}$$

The various wave vectors are given by

$$\vec{k}_c = -K\cos\theta\,\hat{e}_x - q\hat{e}_z = -\vec{k}\,, \tag{25}$$

$$\vec{k}_{cr} = -K\cos\theta\,\hat{e}_x + q\hat{e}_z\,, \tag{26}$$

$$\vec{k}_{ct} = -K\cos\theta\,\hat{e}_x - \bar{q}\hat{e}_z\,, \tag{27}$$

where $K=\omega/c$, and the normal components q and $\bar{q}$ are given by

$$q = K\sin\theta \quad \text{and} \quad \bar{q} = K\left(\sin^2\theta + \chi_0\right)^{1/2}\,. \tag{28}$$

The amplitudes $\vec{\varepsilon}_{cr}$ and $\vec{\varepsilon}_{ct}$ of the reflected and transmitted waves are given by the Fresnel expressions

$$\vec{\varepsilon}_{cr} = r_s\hat{e}_{cr} \quad \text{where} \quad r_s = \frac{q-\bar{q}}{q+\bar{q}}\,\frac{\hat{e}_{cr}\cdot\hat{e}_{ct}}{\hat{e}_c\cdot\hat{e}_{ct}}, \tag{29}$$

and

$$\vec{\varepsilon}_{ct} = t_s\hat{e}_{ct} \quad \text{where} \quad t_s = \frac{2q}{q+\bar{q}}\,\frac{1}{\hat{e}_c\cdot\hat{e}_{ct}}. \tag{30}$$

($\hat{e}_{cr}$ and $\hat{e}_{ct}$ are unit vectors describing the polarization of the specular reflected and transmitted waves.)

Then for a source $\vec{J}_{in}(\vec{r})$ located within the medium, the ART, eq.(15), gives the radiated field as

$$\widehat{e}\cdot\vec{E}(\vec{k}) = -\frac{2\pi}{c}\int_{z<0} \vec{J}_{in}(\vec{r})\cdot\vec{\varepsilon}_{ct}\, e^{i\vec{k}_{ct}\cdot\vec{r}}\, dv\,. \tag{31}$$

On the other hand, had the source $\vec{J}_{out}(\vec{r})$ been located outside the dielectric medium ($z>0$) the corresponding radiated field would be

$$\widehat{e}\cdot\vec{E}(\vec{k}) = -\frac{2\pi}{c}\int_{z>0} \vec{J}_{out}(\vec{r})\cdot\left(\hat{e}_c\, e^{i\vec{k}_c\cdot\vec{r}} + \vec{\varepsilon}_{cr}\, e^{i\vec{k}_{cr}\cdot\vec{r}}\right) dv\,. \tag{32}$$

For an oscillating dipole on the z axis, $\vec{J}(\vec{r}) = -i\omega\vec{p}\delta\left(\vec{r}-z_p\hat{e}_z\right)$, eq.(31) and (32) give

$$\widehat{e}\cdot\vec{E}(\vec{k}) = \begin{cases} 2\pi i K\left(\vec{p}\cdot\hat{e}\, e^{-iqz_p} + \vec{p}\cdot\hat{e}_{cr} r_s\, e^{iqz_p}\right) & \text{if} \quad z_p>0 \\ 2\pi i K\,\vec{p}\cdot\hat{e}_{ct} t_s\, e^{-i\bar{q}z_p} & \text{if} \quad z_p<0. \end{cases} \tag{33}$$

Figure 2: The connecting field for radiation in the presence of a reflecting medium includes reflected and transmitted waves. Here the source $\vec{J}_{in}$ is shown within the medium ($z < 0$).

The power radiated with polarization $\hat{e}$, eq.(18), is

$$\frac{dW}{d\Omega} = \left[\frac{c}{8\pi} K^4 \left(\hat{e} \cdot \vec{p}\right)^2\right] \left|1 + \frac{\hat{e}_{cr} \cdot \vec{p}}{\hat{e} \cdot \vec{p}} r_s \, e^{2iqz_p}\right|^2 \quad \text{for} \quad z_p > 0 \, , \tag{34}$$

and

$$\frac{dW}{d\Omega} = \left[\frac{c}{8\pi} K^4 \left(\hat{e} \cdot \vec{p}\right)^2\right] \left|\frac{\hat{e}_{ct} \cdot \vec{p}}{\hat{e} \cdot \vec{p}} t_s \, e^{-i\bar{q}z_p}\right|^2 \quad \text{for} \quad z_p < 0 \, . \tag{35}$$

In these two expressions we can recognize the first factor (in square brackets) as the power radiated by a dipole in vacuum. The second factor accounts for the presence of the dielectric medium.

4 Specular reflection of polarized x rays

In this section ideas from the three previous examples are combined to study two similar and considerably more involved scattering problems, the specular reflection of polarized x rays by a rough surface and by graded interfaces. We show that within approximations of the Nevot-Croce type grading and roughness affect the specular reflectivity in a manner that is independent of the polarization of the incident radiation.

4.1 Reflection by rough surfaces

The dielectric susceptibility $\chi(\vec{r})$ that describes the rough surface from which we wish to scatter x rays is given by

$$\chi\left(x,y,z\right)=\left\{\begin{array}{lll}0 & \text{for} & z>\zeta(x,y)\\ \chi_0 & \text{for} & z<\zeta(x,y)\end{array}\right. \tag{36}$$

where the height $\zeta(x,y)$, is a Gaussian random variable with zero mean, $\langle\zeta\rangle=0$, and variance $\left\langle\zeta^2\right\rangle=\sigma^2$ (see fig. 3).

To apply the ART it is convenient to rewrite $\chi\left(\vec{r}\right)$ as

$$\chi\left(\vec{r}\right)=\chi_s\left(\vec{r}\right)+\delta\chi\left(\vec{r}\right), \tag{37}$$

where $\chi_s\left(\vec{r}\right)$ represents a medium with an ideally flat surface at z_0,

$$\chi_s\left(\vec{r}\right)=\left\{\begin{array}{lll}0 & \text{for} & z>z_0\\ \chi_0 & \text{for} & z<z_0\end{array}\right. \tag{38}$$

and $\delta\chi\left(\vec{r}\right)$ represents the roughness.

Let $\hat{e}_0\, e^{i\vec{k}_0\cdot\vec{r}}$ be the incident field. The total scattered field $\vec{\varepsilon}(\vec{r})$ includes the wave $\vec{\varepsilon}_s(\vec{r})$ specularly reflected by the step $\chi_s\left(\vec{r}\right)$ plus waves $\delta\vec{\varepsilon}\left(\vec{r}\right)$ scattered by $\delta\chi\left(\vec{r}\right)$

$$\vec{\varepsilon}(\vec{r})=\vec{\varepsilon}_s(\vec{r})+\delta\vec{\varepsilon}\left(\vec{r}\right). \tag{39}$$

The first term on the right is

$$\vec{\varepsilon}_s(\vec{r})=\hat{e}_r\, r_s e^{-2iqz_0}e^{i\vec{k}_r\cdot\vec{r}}, \tag{40}$$

where

$$r_s=\frac{q-\bar{q}}{q+\bar{q}}\,\frac{\hat{e}_r\cdot\hat{e}_t}{\hat{e}_0\cdot\hat{e}_t} \tag{41}$$

($\hat{e}_r$ and $\hat{e}_t$ are unit vectors describing the polarization of the specular reflected and transmitted waves). The second contribution in eq.(39), the field $\delta\vec{\varepsilon}\left(\vec{r}\right)$ includes a specular component plus diffusely scattered and evanescent waves,

$$\delta\vec{\varepsilon}\left(\vec{r}\right)=\delta\varepsilon_r\,\hat{e}_r e^{i\vec{k}_r\cdot\vec{r}}+\delta\vec{\varepsilon}_d(\vec{r}). \tag{42}$$

Using eq.(7) this may be written as

$$\delta\vec{\varepsilon}\left(\vec{r}\right)=\int\frac{d^2k_\perp^{'}}{\left(2\pi\right)^2}\,\frac{K}{k_z^{'}}\delta\vec{\varepsilon}(\vec{k}^{'})\,e^{i\vec{k}^{'}\cdot\vec{r}}, \tag{43}$$

where

$$\delta\vec{\varepsilon}(\vec{k}^{'})=\frac{k_z^{'}}{K}\delta\varepsilon_r\,\hat{e}_r\left(2\pi\right)^2\delta(\vec{k}_\perp^{'}-\vec{k}_{0\perp})+\,\delta\vec{\varepsilon}_d(\vec{k}^{'}). \tag{44}$$

To calculate $\delta\vec{\varepsilon}\left(\vec{r}\right)$ we can proceed exactly as in the previous section (3.3): $\delta\vec{\varepsilon}\left(\vec{r}\right)$ is the field radiated by a current $\delta\vec{J}(\vec{r})$ in the presence of the medium $\chi_s\left(\vec{r}\right)$. The current

$$\delta\vec{J}(\vec{r})=\frac{-i\omega}{4\pi}\delta\chi(\vec{r})\vec{E}\left(\vec{r}\right), \tag{45}$$

Figure 3: The problem of scattering by a rough surface can be tackled using the ART by adding a fictitious overlayer $\delta\chi$.

originates in the polarization of the roughness $\delta\chi(\vec{r})$ by the total electric field $\vec{E}(\vec{r})$ due to the incident and all scattered waves, including those generated by the roughness itself. Thus, the challenge here is that the field $\vec{E}\,(\vec{r})$ is itself unknown; an approximation for it must be obtained as part of our solution.

We can exploit the arbitrariness in the separation of $\chi\,(\vec{r})$ into $\chi_s\,(\vec{r})$ plus $\delta\chi\,(\vec{r})$ to suggest a self-consistent approximation for $\vec{E}$. Suppose we choose z_0 positive and considerably larger than the roughness σ (see fig. 3). Then $\delta\chi\,(\vec{r})$ represents a fictitious overlayer that extends well into the vacuum; the sign of $\delta\chi\,(\vec{r})$ is opposite to that of $\chi_s\,(\vec{r})$ and in the vicinity of z_0 they completely cancel out. The field $\delta\vec{\varepsilon}(\vec{k})$ in a direction $\vec{k}$ with polarization $\hat{e}$ is given by eq.(31)

$$\widehat{e}\cdot\delta\vec{\varepsilon}(\vec{k}) = \frac{iK}{2}\int dv\,\delta\chi(\vec{r})\vec{E}\,(\vec{r})\cdot\vec{\varepsilon}_{ct}\,e^{i\vec{k}_{ct}\cdot\vec{r}}\,, \tag{46}$$

where the connecting field is precisely as in eqs.(24)-(30) except for phase shifts due to the reflecting surface being at z_0,

$$\vec{\varepsilon}_{cr} = e^{-2iqz_0} r_s \hat{e}_{cr} \quad \text{and} \quad \vec{\varepsilon}_{ct} = e^{i(\bar{q}-q)z_0}\, t_s \hat{e}_{ct}. \tag{47}$$

The reason behind the somewhat surprising choice for z_0 will now become clear: slightly above z_0, in vacuum, the exact field is

$$\vec{E}\,(\vec{r}) = \hat{e}_0 e^{i\vec{k}_0\cdot\vec{r}} + \vec{\varepsilon}(\vec{r}) = \hat{e}_0 e^{i\vec{k}_0\cdot\vec{r}} + \vec{\varepsilon}_s(\vec{r}) + \delta\vec{\varepsilon}\,(\vec{r})\,, \tag{48}$$

but slightly below z_0 and, in fact, over all of the extension occupied by $\delta\chi\,(\vec{r})$, we are also in vacuum ($\delta\chi\,(\vec{r})$ and $\chi_s\,(\vec{r})$ cancel each other) and therefore $\vec{E}\,(\vec{r})$ is

given by the same expression (48). The last term $\delta\vec{\varepsilon}\,(\vec{r})$, given by (42), includes some weak diffusely scattered and evanescent waves $\delta\vec{\varepsilon}_d(\vec{r})$. Our approximation consists of neglecting them. Therefore,

$$\vec{E}\,(\vec{r}) \approx \hat{e}_0\, e^{i\vec{k}_0\cdot\vec{r}} + r\hat{e}_r e^{i\vec{k}_r\cdot\vec{r}}, \tag{49}$$

where the specular reflections by $\chi_s\,(\vec{r})$ and $\delta\chi\,(\vec{r})$ have been combined into the single, and still unknown, reflection coefficient r,

$$r = r_s e^{-2iqz_0} + \delta\varepsilon_r. \tag{50}$$

Substituting into eq.(46) yields

$$\widehat{e}\cdot\delta\vec{\varepsilon}(\vec{k}) = -\frac{iK\chi_0}{2}\int dx\,dy\int_{\zeta(x,y)}^{z_0} dz\,\left[\hat{e}_0\, e^{i\vec{k}_0\cdot\vec{r}} + r\hat{e}_r e^{i\vec{k}_r\cdot\vec{r}}\right]\cdot\vec{\varepsilon}_{ct}\, e^{i\vec{k}_{ct}\cdot\vec{r}}. \tag{51}$$

From now on we focus our attention on the specularly reflected component; let $\hat{e} = \hat{e}_c = \hat{e}_r$, $\hat{e}_{cr} = \hat{e}_0$, $\vec{k} = \vec{k}_r = -\vec{k}_c$. Substituting eq.(44) into the left hand side ($l.h.s.$), using $(2\pi)^2\,\delta(k_\perp - k_{0\perp}) = (2\pi)^2\,\delta(0) = \int dx\,dy$ we get

$$l.h.s. = \frac{q}{K}\delta\varepsilon_r\,(2\pi)^2\,\delta(0) = \frac{q}{K}\left(r - r_s e^{-2iqz_0}\right)\int dx\,dy. \tag{52}$$

This shows that the unknown reflection coefficient r we want to calculate appears in both the left and the right hand sides of (51), as part of the radiated field and also as part of the field that induces the source; eq.(51) permits a self-consistent calculation of r.

The integral over dz in the right hand side of eq.(51) is elementary and the remaining integral over $dx\,dy$ is performed using the identity

$$\frac{\int dx\,dy\, e^{-iQ\zeta(x,y)}}{\int dx\,dy} = \langle e^{-iQ\zeta}\rangle = e^{-Q^2\sigma^2/2}, \tag{53}$$

where ζ is a Gaussian random variable with zero mean, $\langle\zeta\rangle = 0$, and variance $\left\langle\zeta^2\right\rangle = \sigma^2$. The right hand side ($r.h.s.$) of eq.(51) becomes

$$\begin{aligned} r.h.s. = \frac{K\chi_0}{2}\left(\int dx\,dy\right)\Bigg\{ & \frac{\hat{e}_0\cdot\vec{\varepsilon}_{ct}}{q+\bar{q}}\,\left[e^{-i(q+\bar{q})z_0} - e^{-(q+\bar{q})^2\sigma^2/2}\right] \\ & -\; r\,\frac{\hat{e}_r\cdot\vec{\varepsilon}_{ct}}{q-\bar{q}}\,\left[e^{i(q-\bar{q})z_0} - e^{-(q-\bar{q})^2\sigma^2/2}\right]\Bigg\}, \end{aligned} \tag{54}$$

which can be further rewritten by substituting $\vec{\varepsilon}_{ct}$ as given by eq.(47), and using $\bar{q}^2 - q^2 = K^2\chi_0$, and

$$\frac{\hat{e}_0\cdot\hat{e}_{ct}}{\hat{e}\cdot\hat{e}_{ct}} = \frac{\hat{e}_{cr}\cdot\hat{e}_{ct}}{\hat{e}\cdot\hat{e}_{ct}} = \frac{\hat{e}_r\cdot\hat{e}_t}{\hat{e}_0\cdot\hat{e}_t} \quad\text{and}\quad \frac{\hat{e}_r\cdot\hat{e}_{ct}}{\hat{e}\cdot\hat{e}_{ct}} = 1. \tag{55}$$

Finally, equating eq.(52) to (54) yields a self-consistent approximation to r,

$$r = \frac{q - \bar{q}}{q + \bar{q}} \frac{\hat{e}_r \cdot \hat{e}_t}{\hat{e}_0 \cdot \hat{e}_t} e^{-2q\bar{q}\sigma^2} = r_s \, e^{-2q\bar{q}\sigma^2}. \quad (56)$$

This coincides exactly with the Nevot-Croce result for the polarization $\hat{e}_0 = \hat{e}_t = \hat{e}_r$ for which the ratio $\hat{e}_0 \cdot \hat{e}_t / \, \hat{e}_r \cdot \hat{e}_t$ is unity, and provides the correct generalization to all polarizations. According to this approximation the specular reflection coefficient r has no polarization dependence beyond that already implicit in the reflection coefficient r_s for the ideal flat step surface; the "static Debye-Waller" factor $exp(-2q\bar{q}\sigma^2)$ is polarization independent.

Notice that any possible dependence on the arbitrary choice of z_0 has cancelled out.

4.2 Reflection by smoothly graded surfaces

The problem of scattering by a smoothly graded interface is similar and somewhat simpler. Here the susceptibility $\chi(z)$ depends only on the normal coordinate z and not on the transverse coordinates x and y. This implies that the tangential component of momentum is conserved in the scattering; there are no diffuse waves, there is only specular scattering.

As before, it is convenient to separate $\chi\,(z)$ into

$$\chi\,(z) = \chi_s\,(z) + \delta\chi\,(z)\,, \quad (57)$$

where $\chi_s\,(z)$ represents an ideally flat surface at z_0,

$$\chi_s\,(z) = \begin{cases} 0 & \text{for} \quad z > z_0 \\ \chi_0 & \text{for} \quad z < z_0 \end{cases} \quad (58)$$

and $\delta\chi\,(z)$ is an overlayer (see fig.4) describing the smooth transition from bulk to vacuum.

Let $\hat{e}_0 \, e^{i\vec{k}_0 \cdot \vec{r}}$ be the incident field. The total scattered field $\vec{\varepsilon}(\vec{r})$, eq.(39),

$$\vec{\varepsilon}(\vec{r}) = \vec{\varepsilon}_s(\vec{r}) + \delta\vec{\varepsilon}\,(\vec{r})\,. \quad (59)$$

includes the wave $\vec{\varepsilon}_s(\vec{r})$ reflected by the step $\chi_s\,(z)$, eq.(40), plus waves $\delta\vec{\varepsilon}\,(\vec{r})$ scattered by the overlayer $\delta\chi\,(z)$. While diffusely scattered waves are not present in $\delta\vec{\varepsilon}\,(\vec{r})$, faint evanescent waves could be; these are weak near field effects and we neglect them. Thus

$$\delta\vec{\varepsilon}\,(\vec{r}) = \delta\varepsilon_r \, \hat{e}_r e^{i\vec{k}_r \cdot \vec{r}}, \quad (60)$$

and the Fourier expansion, eq.(43), and transform $\delta\vec{\varepsilon}(\vec{k})$, eq.(44), remain otherwise unchanged. Once again, $\delta\vec{\varepsilon}\,(\vec{r})$ is radiated by a current

$$\delta\vec{J}(\vec{r}) = \frac{-i\omega}{4\pi}\delta\chi(z)\vec{E}\,(\vec{r})\,, \quad (61)$$

where the field $\vec{E}(\vec{r})$ includes the incident and the unknown reflected waves; $\vec{E}\,(\vec{r})$ must be self-consistently obtained as part of the solution. Then the ART,

Figure 4: The problem of reflection by a graded surface can be tackled using the ART by adding a fictitious overlayer $\delta\chi$. The hatched region shows the transition region from $\delta\chi = 0$ to $\delta\chi = -\chi_0$.

in the form of eq.(31), gives the field $\delta\vec{\varepsilon}(\vec{k})$ in a direction $\vec{k}$ with polarization $\hat{e}$ as

$$\widehat{e}\cdot\delta\vec{\varepsilon}(\vec{k}) = \frac{iK}{2}\int dv\,\delta\chi(z)\vec{E}\,(\vec{r})\cdot\vec{\varepsilon}_{ct}\,e^{i\vec{k}_{ct}\cdot\vec{r}}\,, \tag{62}$$

with the same connecting field given back in eq.(47).

The approximation we use for $\vec{E}\,(\vec{r})$ is the same as in last section. The arbitrariness of z_0 can be exploited by choosing it large enough that the overlayer extends well into the vacuum. Near z_0 the overlayer and the sharp step $\chi_s\,(\vec{r})$ cancel each other out; slightly above z_0, in vacuum, the field is

$$\vec{E}\,(\vec{r}) = \hat{e}_0\,e^{i\vec{k}_0\cdot\vec{r}} + r\hat{e}_r e^{i\vec{k}_r\cdot\vec{r}}, \tag{63}$$

where r is the unknown reflection coefficient we want to calculate,

$$r = r_s e^{-2iqz_0} + \delta\varepsilon_r. \tag{64}$$

Slightly below z_0 and over most of the extension occupied by $\delta\chi\,(z)$ we are also in vacuum (provided the bulk to vacuum transition is not too gradual) and we approximate $\vec{E}\,(\vec{r})$ by the same expression, eq.(63). Substituting into eq.(62) yields an equation for r,

$$\frac{q}{K}\left(r - r_s e^{-2iqz_0}\right)(2\pi)^2\,\delta(k_\perp - k_{0\perp}) =$$

$$= \frac{iK}{2} \int_{-\infty}^{z_0} dz\, \delta\chi(z) \int dx\, dy\, \left[\hat{e}_0\, e^{i\vec{k}_0 \cdot \vec{r}} + r\hat{e}_r e^{i\vec{k}_r \cdot \vec{r}} \right] \cdot \vec{\varepsilon}_{ct}\, e^{i\vec{k}_{ct} \cdot \vec{r}}. \qquad (65)$$

The integral over $dx\, dy$ yields a delta function, $(2\pi)^2\, \delta(k_\perp - k_{0\perp})$, and we can substitute $\hat{e} = \hat{e}_c = \hat{e}_r$, $\hat{e}_{cr} = \hat{e}_0$, $\vec{k} = \vec{k}_r = -\vec{k}_c$. The integral over z is conveniently expressed as

$$\int_{-\infty}^{z_0} dz\, \delta\chi(z)\, e^{-iQz} = \frac{\chi_0}{iQ}[\, e^{-iQz_0} + \frac{\chi'(Q)}{\chi_0}], \qquad (66)$$

where $\chi'(Q)$ is the Fourier transform of $d\chi(z)/dz$,

$$\chi'(Q) = \int_{-\infty}^{+\infty} dz\, \frac{d\chi(z)}{dz}\, e^{-iQz} \qquad (67)$$

Eq.(66) is proved by integrating the left hand side by parts, using $\delta\chi(z_0) \approx -\chi_0$, and $d\delta\chi(z)/dz = d\chi(z)/dz$. Using $\bar{q}^2 - q^2 = K^2\chi_0$ and the identities in eq.(55) the final result is

$$r = r_s\, \frac{\chi'(\bar{q}+q)}{\chi'(\bar{q}-q)}. \qquad (68)$$

Notice that any possible dependence on the arbitrary choice of z_0 has cancelled out.

This coincides exactly with the scalar wave result [17] and provides the correct generalization to all polarizations. Within these approximations the specular reflection coefficient r has no polarization dependence beyond that already implicit in the reflection coefficient r_s for the ideal flat step surface; the "static Debye-Waller" factor is polarization independent.

To conclude we mention some illustrative examples:
(a) The error-function profile

$$\chi(z) = \frac{\chi_0}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{z} dx\, \exp - \left(\frac{x^2}{2\sigma^2} \right), \qquad (69)$$

gives

$$\frac{\chi'(\bar{q}+q)}{\chi'(\bar{q}-q)} = e^{-2q\bar{q}\sigma^2}, \qquad (70)$$

the same factor obtained in the previous section for a Gaussian rough surface. This is as expected, the error function is the averaged profile for the Gaussian rough surface.
(b) The Epstein (or Fermi distribution) profile [17]

$$\chi(z) = \frac{\chi_0}{1 + e^{-z/\sigma}}, \qquad (71)$$

gives

$$\frac{\chi'(\bar{q}+q)}{\chi'(\bar{q}-q)} = \frac{\bar{q}+q}{\bar{q}-q}\, \frac{\sinh[\pi\sigma(q-\bar{q})]}{\sinh[\pi\sigma(q+\bar{q})]}. \qquad (72)$$

(c) The triangular profile

$$\chi(z) = \begin{cases} \chi_0 & \text{for} \quad z < -\sigma/2 \\ \chi_0\,(1 - 2z/\sigma) & \text{for} \quad |z| < \sigma/2 \\ 0 & \text{for} \quad z > \sigma/2 \end{cases} , \tag{73}$$

gives

$$\frac{\chi'(\bar{q}+q)}{\chi'(\bar{q}-q)} = \frac{q-\bar{q}}{q+\bar{q}}\,\frac{\sin[(q+\bar{q})\sigma/2]}{\sin[(q-\bar{q})\sigma/2]}. \tag{74}$$

The reliability of these approximations was studied in [17] in the case of scalar waves. There is no reason to expect any difference from the conclusions reached there: the "static Debye-Waller" in eq.(68) provides a remarkably good approximation for the intensities reflected by interfaces of arbitrary grading profile even for transition regions that are quite wide (σ as large as several nanometers). The phase of the reflected waves is however more sensitive; eq.(68) provides a good approximation for more abrupt transitions (σ of the order of 1 *nm* or less).

5 Conclusion

The main result of this work, eq.(15), is an asymptotic form of the reciprocity theorem which can be used as the basis for a practical method for calculations. The theorem states that the field radiated in the presence of a nontrivial medium, in a certain direction and with a given polarization, is a suitable 'component' of the radiating source. This 'component' is to be extracted by introducing an auxiliary 'connecting' field which contains the necessary information about the medium. The practical advantage of the method lies in the simplifications achieved by systematically avoiding unnecessary calculations; it thereby allows one to tackle problems of increasing complexity.

In forthcoming papers we will further explore the application of the ART to the study of the dynamical diffraction of radiation generated by sources within a crystal, the so-called Kossel lines. Even this well explored topic has not been exhausted. Of particular interest are situations where the Bragg angle lies close to $\pi/2$ and the Kossel cones degenerate into single beams [20], and situations where the source location is revealed by the oscillatory 'Pendellösung' structure of the diffraction pattern [21]. Other applications will include a new approach to thermal diffuse scattering under conditions of dynamical diffraction [22].

Acknowledgments. I am indebted to P. Zambianchi and E. Sutter for valuable discussions.

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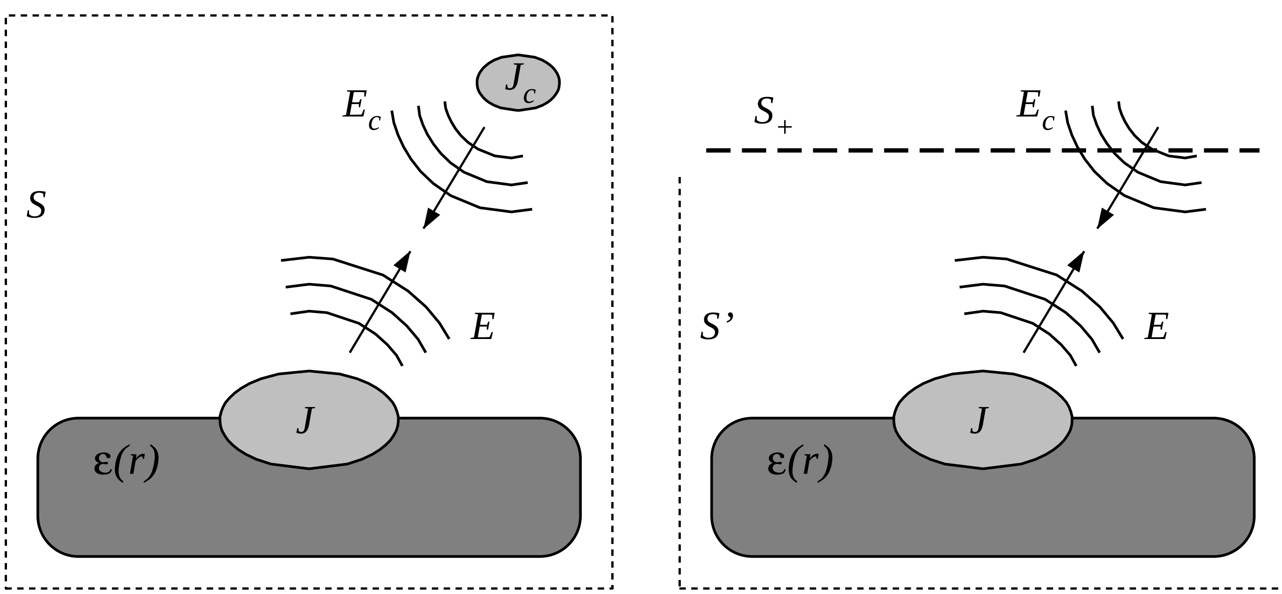
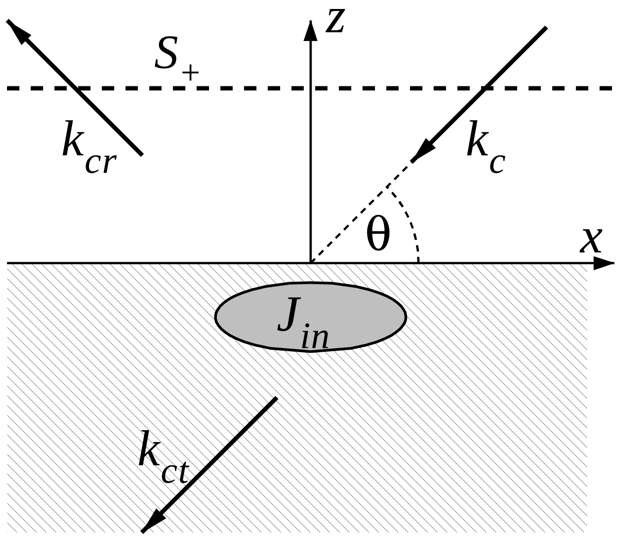
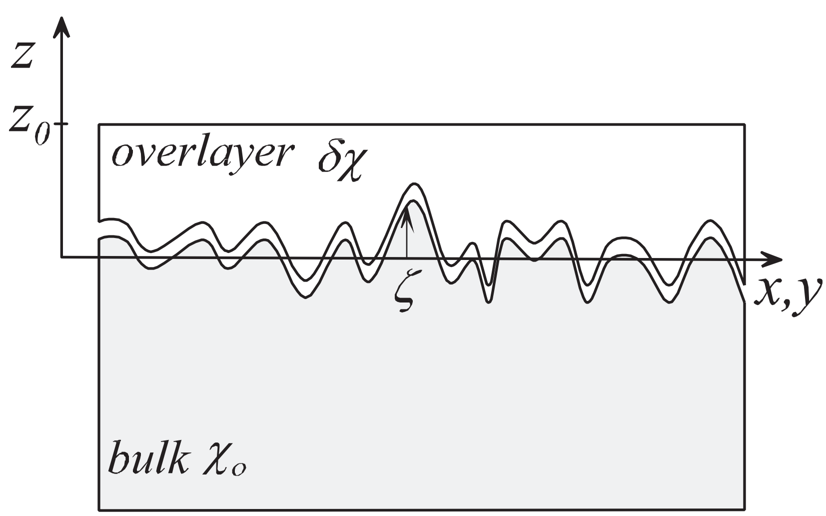


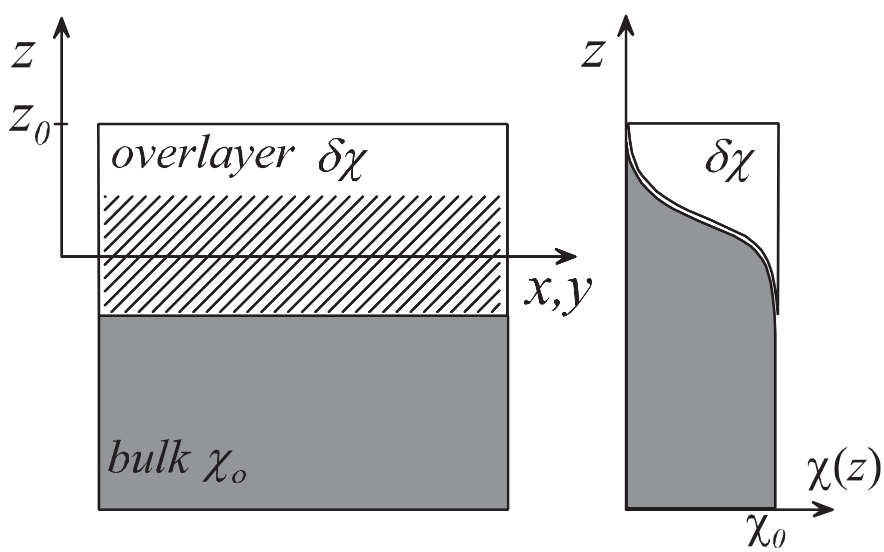
(a) (b)



z
S_+
k_{cr}
k_c
θ
x
J_{in}
k_{ct}



z
z_0
overlayer $\delta\chi$
ζ
x,y
bulk χ_o



z
z0
overlayer δχ
x,y
bulk χo
z
δχ
χ(z)
χ0